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REVIEW ARTICLE

EMERGING TRENDS ON ARTIFICIAL INTELLIGENCE IN PHARMACEUTICALS: A SYSTEMATIC REVIEW

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ABSTRACT:

The frequently use of automation and robotics interchangeably confusing with the term of artificial intelligence (AI). Supercomputer-based AI technology is helpful for determining therapeutics from the molecular structure database. Recently, researchers have applied AI to research and development, general drug discovery, and pharmaceutical manufacturing processes. AI can support scientists with pharmaceutical development and delivery planning, design, quality control, maintenance, and management. In this article, emerging trends on artificial intelligence in pharmaceuticals has been discussed.

KEYWORDS: Artificial Intelligence, Pharmaceuticals, Health Care, Technology.

INTRODUCTION:

Artificial intelligence (AI) is a branch of research that deals with intelligent machine learning, mostly with intelligent computer systems that produce outcomes that resemble human attention. Artificial intelligence (AI) is typically used to analyze machine learning and mimic human cognitive tasks. AI technology is used to obtain meaningful interpretation and to conduct studies

that are more accurate. From this angle, artificial intelligence (AI) technology combines computational intelligence with a variety of practical statistical models. It is likely that the first computer was used in a pharmacy in the 1980s. Since then, computers have been used in a variety of applications, including data collection, clinical research, retail pharmacy management, drug storage, pharmacy education, and much more. With the development of artificial intelligence, it is impossible to predict how much more the pharmacy industry will change over time. Several expert systems have been created in the medical field to help doctors diagnose patients. A number of medication-focused programs have been reported recently.

EMERGING TRENDS ON ARTIFICIAL INTELLIGENCE IN PHARMACEUTICALS:

Aprajita Kimta and Reena Dogra (2024). India's pharmaceutical industry has become a global leader, making substantial contributions to the development of reasonably priced generic medications and vaccines. Notwithstanding its achievements, the industry nevertheless faces difficulties in everything from early R&D to product rollout. The present study investigates the potential benefits and obstacles of incorporating artificial intelligence (AI) into the pharmaceutical industry in India. The study's methodology involves gathering secondary data from 2011 to 2019 from various published sources, particularly the Reserve Bank of India. We evaluated performance using the compound annual growth rate. Artificial intelligence (AI) has promise for resolving long-standing problems, improving operational effectiveness, and lowering medication development and discovery expenses. The public and commercial sectors must work together to ensure successful integration, with a focus on allocating resources for workforce development, infrastructure, education, and regulatory changes. AI integration offers the Indian pharmaceutical industry a game-changing chance to improve drug development, production, and quality assurance. Notwithstanding the encouraging outlook, the report notes that putting AI into practice will present certain difficulties, such as budgetary constraints, labor skill gaps, worries about data security, and regulatory complications. The study highlights the necessity of strategic cooperation to guarantee the ethical and efficient application of AI in the pharmaceutical sector. [1]

Steven Smoke (2024). Though it has received a great deal more attention in the past year, artificial intelligence (AI) is not a novel concept in medicine. As a matter of fact, the FDA had approved close to 700 AI and machine learning (ML)-enabled devices as of 2023. This emphasizes how wide the definition of artificial intelligence is. Specifically, it is the application of models or algorithms to carry out operations and display behaviors like learning, judgment, and prediction. This description makes it understandable that not all AI/ML-enabled technology heralds a revolutionary leap forward in medical science. The list includes, for instance, the 2013-approved Vitek MS (Biomerieux) microbial identification system. Despite its crucial role in clinical care, doctors analyzing the instrument's results may not readily recognize the use of AI in this tool. [2]

Abou Hajal, A., and Al Meslamani, A. Z. (2024). Artificial intelligence (AI) is transforming the drug development business with the promise of increased efficiency, lower prices, and higher success rates due to the expansion of chemical and biological data. Applications of artificial intelligence include target identification and validation, hit discovery, lead prioritization, drug property prediction, de novo drug design, chemical synthesis, and drug repurposing. Despite these significant advancements, researchers continue to explore the full potential of AI, ML, and DL in drug development, especially in balancing the current need for accuracy with the unpredictable nature of early findings. This editorial describes the state of AI in drug discovery now, evaluates its promise and capabilities, and projects where it will go in the future. AI tools provide robust techniques for methodically analyzing intricate biological information to find, rank, and assess druggable, safe, and effective candidate targets. [3]

Tade RS et al. (2024). Artificial intelligence has become a game-changer in the biomedical and pharmaceutical industries. This review delves into its disruptive influence in the pharmaceutical sector, specifically in drug development and future intervention discovery. These procedures are now more productive, economical, and able to provide patients with customized care because of the use of AI. Furthermore, since AI can scan large datasets for important patterns and trends, it holds great potential for disease prevention and outbreak prediction, enabling the customization of actions to combat disease. AI has proven to be extremely helpful in biomedical research, particularly in the fields of genomes, proteomics, and metabolomics, where it allows scientists to thoroughly examine complicated biological data, leading to the discovery of new information and

hastening scientific progress. The patient-physician interface is another area where AI has an impact because it improves treatment efficiency and diagnosis precision, which in turn leads to better patient care. [4]

Yashvi Thakor and Gufran Ahmad Ansari (2024). An era of transformation in patient care and medical research has been sparked by the use of artificial intelligence (AI) in healthcare and medication development. This study looks at how the drug development industry is changing and emphasizes how important artificial intelligence is to improving healthcare for people. AI has the potential to revolutionize the fields of target identification, molecular screening, lead optimization, and clinical trial design by fusing data-driven methodologies with cutting-edge machine learning algorithms. AI applications in healthcare promise improved patient care, lower costs, and advancements in medical research. These applications include medical image analysis, illness diagnosis, tailored treatment, electronic health information management, and more. Nevertheless, there are drawbacks to these developments, including concerns about bias, data protection, legal restrictions, and morality. The essay examines comparable AI-based approaches and solutions, while also highlighting the potential of AI in medication development and healthcare. We also cover concerns like data security, interoperability, quality, regulatory approval, ethical concerns, and resource limitations. For healthcare AI solutions to be safe and effective, responsible development and deployment are essential. In the future, efforts will focus on enhancing explainability, encouraging information exchange and teamwork, developing ethical frameworks, modifying regulatory procedures, incorporating AI into clinical practice, and tackling inequalities in global health. AI has the potential to completely transform healthcare through cooperation and ongoing research, improving patient outcomes and paving the way for a more promising future for medicine. [5]

Fang Bai et al. (2024). The emergence of the third wave of artificial intelligence (AI) is ushering in a new chapter in drug development. In biomedical research, AI-powered methods have the potential to uncover features from large, high-dimensional data that are challenging for humans to understand. This explains the intense interest in artificial intelligence (AI) in drug discovery, both in academia and industry. The drug discovery process is undergoing a revolution thanks to the proliferation of AI tools, which also have the potential to significantly alter the industry's

economics and pace. Our earlier analysis offered a thorough rundown of the advancements in this field. [6]

Yizhen Luo et al. (2024). Human specialists usually learn about the molecular properties of medications and proteins in the real world through a variety of multimodal sources, such as molecular structures, organized knowledge from knowledge bases, and unstructured knowledge from biomedical literature. The current multimodal approaches in artificial intelligence drug development undermine the comprehensive understanding of biomolecules by integrating either structured or unstructured knowledge individually. Furthermore, they do not deal with the issue of missing modality, which is the lack of multimodal information for novel medicines and proteins. Here, we introduce KEDD, a comprehensive, end-to-end deep learning system that combines organized and unstructured data for large-scale AI drug discovery applications. Initially, the structure integrates autonomous representation learning models to derive the fundamental attributes from every modality. It then uses a feature fusion technique to determine the outcome of the prediction. We use modality masking and sparse attention to recreate the missing features based on the most important molecules in order to lessen the impact of the missing modality issue. By utilizing both organized and unorganized information, our framework expands our understanding of biomolecules. In terms of drug-target interaction prediction, drug property prediction, drug-drug interaction prediction, and protein-protein interaction prediction, KEDD outperforms the most recent models by an average of 5.2%, 2.6%, 1.2%, and 4.1%, respectively. We demonstrate the promising potential of KEDD in supporting real-world applications through qualitative analysis. KEDD shows promise for expediting drug discovery by integrating multimodal information with biomolecular understanding. [7]

Bhattamisra SK et al. (2023). Artificial intelligence (AI), a subfield of computer science, enables robots to analyze complex data and operate more productively. AI-focused research has grown significantly, and its application to healthcare services and research is developing at a faster rate. This paper delves into the advantages and challenges of AI in medical and pharmaceutical research. Using specific keywords and phrases like "artificial intelligence," "pharmaceutical research," "drug discovery," "clinical trial," "disease diagnosis," etc., the literature was gathered from domains like PubMed, Science Direct, and Google Scholar in order to select and review

articles published within the last five years. This article discusses in great detail the use of AI in disease diagnostics, digital therapy, individualized treatment, drug discovery, and pandemic or epidemic forecasting. The most popular artificial intelligence (AI) technologies are deep learning and neural networks; prospective technologies for clinical trial design are Bayesian nonparametric models; wearable technology and natural language processing are employed for patient identification and clinical trial monitoring. We utilized deep learning and neural networks to predict the outbreaks of COVID-19, Zika, Ebola, and seasonal influenza. The scientific community may see quick and affordable advances in pharmaceutical and healthcare research, as well as better public services, thanks to the development of AI technologies. [8]

Vora, Lalitkumar K., et al. (2023). Artificial intelligence (AI) has become a potent instrument that utilizes personal knowledge and offers quicker fixes for difficult problems. Promising developments in artificial intelligence and machine learning offer a game-changing prospect for drug discovery, formulation, and dosage form testing. Through the application of AI algorithms that examine vast amounts of biological data, such as proteomics and genomics, scientists are able to pinpoint targets linked to disease and anticipate how those targets may interact with possible therapeutic candidates. This makes it possible to approach drug discovery in a more effective and focused manner, which raises the possibility of successful drug approvals. Additionally, by streamlining research and development procedures, AI can help lower development costs. The pharmacokinetics and toxicity of potential drugs can be predicted using machine learning algorithms, which also help with experimental design. This capacity reduces the need for extensive and expensive animal research by allowing lead compounds to be prioritized and optimized. Artificial intelligence (AI) algorithms that evaluate real-world patient data can support personalized medicine strategies, improving patient adherence and treatment outcomes. This thorough overview examines the broad range of uses of AI in drug discovery, drug delivery dosage form designs, process optimization, testing, and pharmacokinetics/pharmacodynamics (PK/PD) investigations. This analysis highlights the advantages and disadvantages of the several AI-based techniques used in pharmaceutical technology. However, the pharmaceutical industry's ongoing exploration and investment in AI present great opportunities for improving patient care and drug development procedures. [9]

Sultana, A. et al. (2023). The review covers a wide range of subjects connected to artificial intelligence (AI) in drug development. It also provides a brief summary of the latest developments in medication research produced by the pharmaceutical sector in collaboration with different AIs. Technological and computational advancements have influenced scientific fact. Artificial intelligence has become an essential component in every aspect of science and technology, ranging from basic engineering to medicine. AI has had such an impact on medical science and pharmaceutical chemistry. In recent years, the use of computers to aid in the production of drugs has surpassed more traditional methods. Artificial intelligence is widely employed to expedite and enhance medication design procedures. AI significantly increases the success percentage of the produced medication by simplifying the identification of target proteins. Artificial intelligence (AI) is used at every stage of the pharmaceutical design process, resulting in reduced costs and health risks associated with preclinical research. Large-scale pharmaceutical data sets and machine learning are the foundation of artificial intelligence (AI), a potent data mining approach. The result is the use of AI in de novo drug design, activity scoring, virtual screening, and in silico assessment of drug molecule properties (absorption, distribution, metabolism, excretion, and toxicity). Pharmaceutical corporations have partnered with AI firms to accelerate drug research and the healthcare system. [10]

Sakshi V. Dashpute et al. (2023). Artificial intelligence (AI) has revolutionized several aspects of the pharmaceutical sector, including marketing, clinical trials, manufacturing, and medication research and development. AI can do everything from reducing mistakes and increasing accuracy to opening up previously unthinkable new ideas. The pharmaceutical industry is using AI to produce new drugs. Some of the applications of this technology include optimizing medication designs and predicting molecular structures. AI also helps with drug repurposing by locating drugs for new medical applications swiftly and affordably. AI-driven automation in manufacturing streamlines processes, enhances quality assurance, and maximizes production parameters. Advanced process control and fault detection enable efficient production, while artificial intelligence-driven trend analysis assists in identifying and resolving potential issues. AI is useful in clinical trials because it helps with patient recruitment, data processing, and monitoring—an essential phase of drug research. The use of AI algorithms to predict trial results and diagnose medical conditions holds great promise for enhancing patient care and trial success rates. The

pharmaceutical business faces challenges in adopting AI despite its many benefits, including high initial costs, worries about job loss, and limitations in data collection. Given its potential to transform drug development procedures and improve patient outcomes, artificial intelligence is expected to have a substantial impact on the pharmaceutical sector in the near future. AI's incorporation into the pharmaceutical sector is a huge step forward, providing a host of advantages while tackling the complexities and difficulties of contemporary medicine and drug development. [11]

Mingkun Lu et al. (2023). Drug research and development significantly impacts the pharmaceutical industry and impacts many facets of human health. However, because medication research and development (R&D) is a drawn-out and intricate process, investments in novel drugs sometimes yield no returns. Artificial intelligence (AI) has become a major tool for evaluating large amounts of high-dimensional data in recent years due to advancements in computer hardware and experimental technology. The size of biological data is growing at an explosive rate, which offers benefits for using AI in all phases of pharmacological R&D. AI's capacity to find novel treatments more quickly and cheaply has revolutionized drug research and development, driven by big data in biomedicine. This review starts with a quick synopsis of popular AI models used in drug discovery. It then goes into great detail about each model's unique uses in different phases of drug R&D, including target identification, drug discovery and design, preclinical research, automated drug synthesis, and market impacts. Lastly, it provides a thorough discussion of AI's main shortcomings in drug research and development, along with potential fixes. [12]

Hansa Choudhary et al. (2023). Artificial intelligence (AI) finds increasing use across several domains in society, especially in the pharmaceutical industry. AI has benefits for both professionals and the economy. By mimicking human intelligence and fusing it with state-of-the-art technology, it reduces the need for human labor and produces the best outcomes. This paper looks at the practical usage of AI in the pharmaceutical business across multiple departments and at every stage, from drug discovery to medication development. It reduces the need for human labor, improves pharmaceutical output and clinical research efficacy, and lowers the risk of error. The analysis also examines the challenges that the pharmaceutical industry is now facing in deploying AI. It also evaluates present issues and makes recommendations for fixes. [13]

Prasad Patil et al. (2023). Artificial intelligence has the ability to completely change a wide range of pharmaceutical industry-related elements. In this article, we give a summary of the advantages and uses of AI in the pharmaceutical sector, including topics such as personalized medicine, clinical trial design, drug discovery, expediting drug development, and improving medication safety. We have also explored the effects of artificial intelligence and its instruments on the pharmaceutical sector, and the significant global start-ups in this field. However, the pharmaceutical sector must overcome a number of obstacles before it can widely use AI. These include unclear regulatory guidance, worries about data security and privacy, problems with data availability and quality, and ethical dilemmas. Despite these obstacles, ongoing research and development in AI has the potential to greatly increase patient outcomes as well as the effectiveness and precision of drug development. In conclusion, while AI holds immense potential for the pharmaceutical sector, its full realization still requires the removal of numerous obstacles. [14]

Blanco-González A et al. (2023). Artificial intelligence (AI) has the potential to completely transform the process of finding new drugs by offering increased speed, accuracy, and efficiency. However, the availability of high-quality data, the resolution of ethical issues, and the understanding of the limitations of AI-based methods are necessary for the successful implementation of AI. This article reviews the advantages, difficulties, and disadvantages of artificial intelligence (AI) in this subject and suggests some potential solutions and tactics for getting beyond the current roadblocks. We also cover the application of explainable AI, data augmentation, and AI integration with conventional experimental techniques, along with the potential benefits of AI in pharmaceutical research. In summary, this study sheds light on the potential applications of artificial intelligence (AI) in drug discovery and discusses the obstacles and prospects associated with doing so. A note from the authors: This article aimed to assess ChatGPT's (a chatbot based on the GPT-3.5 language model) ability to assist human authors in writing review articles. We assessed the AI's capacity to automatically generate material using the text it produced after receiving our instructions (see Supporting Information). The human writers essentially updated the text after carrying out a comprehensive review, making an effort to preserve

harmony between the initial concept and the scientific standards. The final section discusses the benefits and drawbacks of applying AI in this way. [15]

Sarika Bhabad et al. (2023). Within computer science, artificial intelligence (AI) is a specialized field that enables machines to process and interpret complex data quickly. AI-related research has been rapidly expanding, especially in its application to healthcare services and research. This paper explores the many potentials and difficulties that artificial intelligence (AI) brings to the fields of pharmaceutical research and healthcare. We conducted a thorough search using databases such as PubMed, Science Direct, and Google Scholar to gather pertinent literature. This article covers in detail the use of AI in several healthcare domains, including disease diagnosis, digital therapy, individualized treatment, drug development, and pandemic or epidemic prediction. Artificial intelligence mostly uses deep learning and neural networks. The assessment highlights how important it is for AI technologies to advance in order to support quick and affordable pharmaceutical and healthcare research. Better service delivery to the general population is the expected result, which reflects AI's revolutionary influence on scientific pursuits. [16]

Niyati Shah (2023). Artificial intelligence (AI) has become increasingly prevalent in pharmaceutical technology, and it has the potential to reduce costs and save time while also enhancing our comprehension of the relationships between different formulations and process variables. Artificial intelligence (AI) is a branch of computer science that uses symbolic programming to solve problems. It has evolved into a science of problem solving with broad applications in engineering, business, and medicine. The creation of unique peptides from whole foods, the management and treatment of uncommon illnesses, dose and adherence to medication, and obstacles to AI's widespread use in pharmaceuticals are all covered in this article. AI to forecast new treatments, automated control process systems, and manufacturing execution systems are also covered. [17]

Parvathaneni M. et al. (2023). Historically, drug discovery has been a costly and time-consuming process. Furthermore, the drugs were not as well-designed as they are now, thanks to AI and ML prediction and development. More recently, machine learning—a type of artificial intelligence that grows and changes depending on experience, much like the human mind—has been applied to the

creation and discovery of new drugs. Better dosage formulations, reduced toxicity, and more target precision have all been made possible by the incorporation of AI and ML into the drug discovery and development process. Generally speaking, artificial intelligence (AI) has been introduced and used at every stage of the drug development process, from hit discovery and validation to target identification and hit-to-lead optimization. This has greatly shortened the formerly drawn-out drug screening procedure. Additionally, downstream in the medication formulation process, AI and ML have been used to optimize resource efficiency and enable web-based 3D printing of pharmaceuticals. The modeling of novel drug-like molecules to forecast their ADMET properties is another way that artificial intelligence is being used in the drug development process. The phases of drug discovery and development where the use of AI and ML modeling has changed the conventional drug development process will be covered in this paper. [18]

Shivani Agarwal et al. (2023). This review paper served as a helpful, brief introduction to artificial intelligence for physicians and pharmacists. Here, we discuss the applications of AI in healthcare, including its benefits and drawbacks for pharmacists, as well as its instruments. It has applications in many different industries, including business, pharmacy, health care, and engineering, and has significantly advanced into decision-making, problem-solving, and critical thinking. [19]

Raza, Muhammad Ahmer, et al. (2022). Artificial intelligence (AI) has become a popular remedy for issues involving numbers and data. Numerous technological advances have resulted from this discovery in almost every industry, including engineering, architecture, education, business, accounting, health, and so forth. AI has made significant contributions to the healthcare industry in a number of areas, including the management and storage of data and information about patient medical histories, medication stocks, sale records, and more; automated machinery; software and computer applications; and diagnostic tools like CT and MRI diagnostics. All of these have been developed to support and streamline healthcare procedures. Without a doubt, artificial intelligence (AI) has transformed healthcare to be more effective and efficient, and the pharmaceutical industry is not exempt. In recent years, there has been a discernible surge in interest in the application of AI technology for the analysis and interpretation of several significant pharmacy domains, including drug development, dosage form design, polypharmacology, and hospital pharmacy. We intended to produce a thorough report that would aid every practicing pharmacist in understanding

the major advancements made possible by the application of artificial intelligence (AI) in light of the field's expanding significance. [20]

Kolluri, S. et al. (2022). In the last ten years, machine learning (ML) and artificial intelligence (AI) have emerged as the game-changing technologies most likely to revolutionize pharmaceutical research and development (R&D). This is partly due to the dramatic developments in computational technology, as well as the concurrent dismantling of earlier limitations on the gathering and processing of massive amounts of data. In the meantime, it is now unaffordable to introduce new medications to patients and the market. Despite these challenges, the pharmaceutical business finds AI/ML systems attractive because of their automated nature, predictive power, and anticipated boost in efficiency. The drug development process has applied ML techniques with increasing sophistication over the past 15–20 years. The most recent area of drug development where AI/ML is beginning to have a positive impact in the planning, execution, and analysis of clinical trials. Because clinical trial conduct is increasingly dependent on digital technology, the COVID-19 pandemic may expedite the use of AI and ML in clinical trials. It's imperative to cut through the noise and buzzwords surrounding AI and ML as we head toward a world where its use in R&D is expanding. Recognizing that the scientific process is still applicable when drawing conclusions from evidence is crucial. This will make it easier to distinguish reality from fiction and make wise decisions on how best to apply AI and ML to the drug development process. This book seeks to provide a balanced perspective on the best use of AI and ML techniques in research and development by demystifying important ideas and presenting use-cases. [21]

Patel S.S., Shah S.A. (2022). The goal of artificial intelligence (AI) is to create intelligent modeling that facilitates knowledge conception, problem solving, and decision-making. Warren McCulloch and Walter Pits conducted the initial research known as artificial intelligence (AI) in 1943. Artificial intelligence (AI) was once thought to be exclusive to the engineering domain. However, the pharmacy industry now widely uses AI in various domains such as drug discovery, drug delivery formulation development, marketing, management, quality assurance, and hospital pharmacy. Many artificial neural networks (ANNs), such as deep neural networks (DNNs) or

recurrent neural networks (RNNs), are used in drug discovery and drug delivery formulation development. Currently, a number of drug discovery implementations have been examined, and the technology's potential in quantitative structure-property relationship (QSPR) or quantitative structure-activity relationship (QSAR) has been validated. Furthermore, de novo design encourages the development of substantially noveler pharmacological molecules in terms of desired or ideal characteristics. Nowadays, doctors use robots for a variety of medical operations because they are more reliable than humans, have more advanced job capabilities, and can complete any task quickly and efficiently. We conclude that artificial intelligence (AI) is the new, developing field in every industry, including pharmacy, and that it needs further development in order to update the state of the art and conduct new research. [22]

Pareek, Varun et al. (2022). The fourth industrial revolution is frequently hailed as being ushered in by artificial intelligence (AI), which is expected to play a significant role in practically every area of our society. This makes it imperative to assess the advantages and drawbacks of artificial intelligence (AI) and machine learning (ML) in a variety of industries. Although the pharmaceutical business has been a leader in implementing AI in all of its key areas, its current level of success appears to be quite low. The main benefit of artificial intelligence (AI) is that it shortens the time required for medication development, which lowers related expenses, increases return on investment, and may even result in lower end-user costs and increased drug safety. Therefore, in addition to a quick overview of how AI and ML may affect geriatric health care, we will also examine the extent and constraints of AI in the pharmaceutical business in this article. [23]

Veer Patel and Manan Shah (2022). Machine learning and artificial intelligence have advanced significantly in recent years. It has greatly raised the quality of life while decreasing human burden. This article uses artificial intelligence and machine learning to enhance the efficiency and accuracy of drug research and development. This research conducted a systematic review of papers, which were chosen based on the authors' existing knowledge and a keyword search in publicly accessible databases. We filtered the results based on relevant context, abstract, methodology, and full text. A body of work has supported the roles of machine learning and artificial intelligence in facilitating drug development and discovery processes due to the ability to conduct simulations with these

technologies. This has included making these processes more cost-effective or completely eliminating the need for clinical trials. Additionally, they made it possible for scientists to thoroughly examine various chemicals without the need for trials. The results of this study demonstrate how common machine learning and artificial intelligence techniques are in the field of drug discovery and point to a bright future for these technologies. As a result, scholars, students, and the pharmaceutical industry will be able to learn more about machine learning and artificial intelligence in the context of drug development and discovery. [24]

K. Soni and Y. Hasija (2022). Artificial intelligence, or AI for short, is defined as a group of interconnected technologies that enable robots to see, comprehend, act, and learn at a level of intelligence comparable to that of humans. The AI area includes technologies such as machine learning (ML) and natural language processing (NLP). All these are in different stages of development, but when paired with computerization, analytics, and datasets, they could help organizations accomplish their goals, whether they are supply chain optimization or customer service improvement. The process of developing new medications is not only complex but also quite expensive and time-consuming. This process takes about 12 years on average and costs about 2.6 billion USD. Artificial intelligence (AI)-based approaches are employed at nearly every stage of the drug discovery and development process in this era of increased computer capacity. AI has sped up the entire process of developing new pharmaceutical breakthroughs by lowering the time and financial requirements involved. In this book, we've covered a few of the most significant uses of AI in the pharmaceutical industry. It has also been discussed how researchers utilize several tools, including Toxtree, ADMET, ProTox, and others, to predict the toxicity of pharmaceuticals during the drug discovery process. We have also discussed how AI is turning out to be a potent weapon in the fight against the COVID-19 pandemic, such as in genomes, vaccination, and detection of the SARS-CoV-2 virus. Furthermore, we have talked about how the introduction of AI-powered businesses into the pharmaceutical industry has led to some noteworthy achievements. For example, DeepMind's AlphaFold2 has predicted the three-dimensional structure of proteins, and Insilico Medicine's Chemistry42 has identified a novel drug candidate for kidney fibrosis. We've also discussed the promising future AI is predicted to bring about in the pharmaceutical industry, with a particular emphasis on drug research. [25]

Praveen Tahilani et al. (2022). The Era of Artificial Intelligence, Machine Learning, and Data Science in the Pharmaceutical Industry is a developing field that emphasizes how new technologies have increased effectiveness in the drug discovery process. As things stand, machine learning and artificial intelligence may be the future for many fields and businesses, most notably the pharmaceutical sector. The pharmaceutical industry places great importance on reducing costs and time, given that a single authorized drug currently costs the corporation millions of dollars and necessitates years of rigorous testing before obtaining a license. Artificial intelligence will be helpful to the pharmaceutical sector, and researchers in the fields of chemical biology, computational chemistry, medicinal chemistry, and bioinformatics will find it interesting. [26]

More Swati K. (2022). Artificial intelligence in medicine is the next frontier in the biological sciences. Artificial intelligence is a subfield of computer and engineering sciences that possesses the ability to solve problems. In essence, artificial intelligence is a machine-learning program that is desperately needed in the pharmaceutical sector these days. In the drug discovery sector of pharmaceutical research and development, it should be necessary to forecast the development of new drug molecules. It should also be much more necessary in studies that evaluate medications and other biological molecular models. Artificial intelligence may also speed up the clinical trial and medication discovery processes, as well as lead to additional research. [27]

F. I. Saldívar-Gonzále et al. (2022). Natural products (NPs) are special structures that interact with protein therapeutic targets, according to the main understanding. Even though the pharmaceutical industry has mostly given up, its distinctive qualities and structural variety continue to amaze scientists for their ability to generate treatments inspired by natural products. The advancements in computer technology, storage capacity, software accessibility, and low-cost online education, many industries and research fields now widely use artificial intelligence (AI). In order to address obstacles in NP drug development and create new opportunities, two subfields of artificial intelligence (AI) have emerged in recent decades: natural language processing and machine learning algorithms. This paper looks at and talks about the useful ways that AI techniques were made to help find bioactive natural products (NPs) and figure out the "patterns" of these special structures for choosing targets or designing combinations. [28]

V Kalayil et al. (2022). Drug discovery is a complex problem that requires enhancing several aspects of drug candidates, including safety, pharmacokinetics, and efficacy, to produce the final drug product. Recent developments in areas such as artificial intelligence (AI) systems, which enhance the design thesis through report investigation, microfluidics-assisted chemical synthesis, and biological testing, are laying the foundation for further automation of this process. AI has made drug discovery with computers easier. This may enable more fruitful searches for related compounds, reducing the time it takes to identify and improve compounds. But this kind of optimization also gives rise to more substantive philosophical, technological, and organizational questions and mistrust regarding the continuous acceleration surrounding them. Global advancements in machine learning, particularly deep learning, across several scientific fields and advancements in computer hardware and software are some of the driving forces behind this growth. [29]

Adam Zielinski (2021). This study looks at how advances in pharmaceutical artificial intelligence (AI) could impact the creation of new medications in the years to come. A wide range of sources, including industry literature, research journals, AI studies, market reports, market projections, discussion papers, news releases, and the websites of organizations, were examined in order to provide an answer to the topic. The study makes the case that ongoing advancements in pharmaceutical AI will hasten the creation of secure and efficient treatments for illnesses that were previously incurable. A number of important points support this conclusion. AI-enabled research methodologies can be immediately utilized to lower the time and cost of drug discovery projects. The pharmaceutical sector is currently experiencing a severe productivity crisis. The pharmaceutical sector has already released data, including a ten-fold decrease in therapeutic compound discovery timeframes. Many AI partnerships between government, business, and academia made it possible to use proprietary data, which produced results like the most comprehensive database of molecular toxicity ever created or more than 200 medication safety prediction models. Record-breaking fundraising rounds and the participation of tech titans have recently accelerated the momentum. Long-term effects will include new commercial strategies focused on diseases that are now incurable, large-scale collaboration, safer and more effective medications, and a reduction in the importance of pharmaceutical patents. Even a small portion of these advancements might help ease the productivity crisis, the research observes, despite the fact

that many of the evaluated resources appear to have unduly optimistic future expectations. Ultimately, the study comes to the conclusion that the industry's emphasis on pharmaceutical AI sets it up for yet another big disruption: open data sharing and cooperation. [30]

Yamini D Shah et al. (2021). The branch of science and engineering known as artificial intelligence (AI) is defined as focusing on creating fascinations that exhibit cautious behavior and creating artificial intelligence that can recognize and understand them. Artificial intelligence (AI) is a broad term that encompasses a number of developments, many of which have been in development for some years, with the goal of using human-like reasoning to solve problems. As a result of the massive increase in processing capacity and the substantially larger increase in information, we are currently witnessing a revived enthusiasm for AI in conjunction with upgraded advances that are either extreme or significantly more involved. Machine learning and computer vision can both benefit from AI applications. These future possibilities can lead to greater global benefits in the fields of engineering and medicine. The healthcare sector is the next industry to experience the impact of artificial intelligence. AI treats critical illnesses like diabetes, cancer, neurology, and cardiology. The review includes the ongoing flow status of medical services for AI applications. There are a few forward-thinking investigations into AI applications in healthcare that offer an outlook on a future in which social insurance conveyance progressively bridges human relationships. In a similar vein, this review will cover how AI and machine learning can save lives. It can be used as a guide for healthcare practitioners to determine how, when, and where AI can be more effective and produce the intended results. [31]

Sudipta Das et al. (2021). The goal of artificial intelligence (AI) is to create intelligent modeling that facilitates knowledge conception, problem solving, and decision-making. These days, artificial intelligence (AI) is a major factor in many pharmacy domains, including polypharmacology, hospital pharmacy, drug discovery, and drug delivery formulation development. Drug discovery and drug delivery formulation development use many artificial neural networks (ANNs), such as deep neural networks (DNNs) or recurrent neural networks (RNNs). Researchers have currently examined a number of drug discovery implementations, demonstrating the technology's effectiveness in determining quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). Furthermore, de

novo design encourages the development of substantially noveler pharmacological molecules in terms of desired or ideal characteristics. The current review paper covers the uses of AI in pharmacy, focusing on polypharmacology, hospital pharmacy, drug delivery formulation development, and drug discovery. [32]

Maithri H. Shanbhogue et al. (2021). In practically every subject, artificial intelligence is a developing field. Technology, health, and research are just a few of the industries in which it can find application. Artificial intelligence primarily focuses on how computers digest information and simulate human reasoning. Artificial intelligence can be one potential way to get around the high R&D expenditures and unpredictable time consumption associated with drug development. Because of the abundance of available data, it is possible to overlook certain important information. We are using algorithms such as machine learning, deep learning, and other expert systems to address these issues. The pharmaceutical industry can minimize failures in clinical and marketing settings and delays in drug development by effectively applying AI. This overview provides details on the history of artificial intelligence (AI), its various subfields, its general applications, and its application in the pharmaceutical industry. It also offers insights into the difficulties and constraints associated with AI. [33]

Jürgen Bajorath et al. (2020). Recommendation-based computer systems are becoming more common in our daily lives. E-commerce websites, for instance, offer suggestions based on our past purchases. Online streaming services suggest videos and music that we might like. An article that appears in this issue applies this concept to the medicinal chemistry lab. The authors explain how it is possible to use the idea that "people who bought this also bought this" to suggest tests that could yield further information, three-dimensional structures of related substances, and methods for organic synthesis. [34]

Manoj K Chaudhari and Vipul P Patel (2020). The area of computer science known as artificial intelligence focuses on using symbolic programming to solve problems. Artificial intelligence has enormous potential for solving health-related issues. The creation of expert systems is a significant and practical use for artificial intelligence. The artificial intelligence, doctors can now operate with accuracy and reliability. Many institutions are using robots to carry out specific tasks under human

supervision. One of the main benefits of artificial intelligence is that it shortens drug development time, which reduces costs and saves time. Numerous studies are underway to enhance the effectiveness of the pharmacy profession. This article elucidates the role of artificial intelligence in medication development and the technologies employed in this process. [35]

CONCLUSION:

The latest advancements in AI have captivated researchers, particularly in the areas of healthcare and pharmaceutical research and services. The future of the healthcare industry will be shaped by smart hospitals and healthcare facilities that are equipped with AI, ML, and big data. Artificial intelligence (AI) has promise for reducing the time and cost associated with medication development as the pharmaceutical industry continues to expand its technological capabilities. Through the use of deep learning, neural networks, and unsupervised learning, the importance of AI in disease detection is clearly illustrated. These artificial intelligence (AI) tools are effective for diagnosing specific diseases because they can process unstructured data and link it with learned data to anticipate an accurate conclusion. Intelligent computer-assisted instruction (ICAI), case-based reasoning, vector regression analysis, and clinical decision support—all of which use AI to track the progression of chronic diseases and optimize treatment—have all been shown to be essential technologies. The vector regression technique is helpful in determining the relationships between variables; ICAI is helpful in providing computer-assisted instruction to patients in order to obtain an informative response from the patients; case-based reasoning aids in problem solving by drawing on prior experiences of a kind; and clinical decision support gives the healthcare team patient-specific knowledge and information to aid in disease monitoring and treatment. The development of personalized treatment, which is always difficult, is made easier by these technologies. Additional methods like high-resolution retinal imaging and radiomics, which forecast the results and toxicity of radiation therapy for specific individuals, provide further opportunity to study human health. The main goal of pharmaceutical R&D, which is an expensive and time-consuming process, is drug discovery and the introduction of new drugs to the market. AI has the ability to streamline the entire process, from drug clinical trials to target selection. The first step in the drug discovery process is to identify the target biological substances that obstruct the disease's modification. Thousands of synthetic compounds are produced during the drug

development process with the potential to attach to the target and change its function in order to manage a certain disease. The physicochemical and pharmacokinetic qualities are ascertained in this manner by the use of computer-aided drug design and quantitative structure-activity relationships (QSAR) or quantitative structure-property relationships (QSPR). The prediction of lipophilicity and solubility of an NCE is done using deep learning and neural networks that are based on the ADMET predictor and ALGOPS program. The artificial intelligence tools that forecast drug-target interactions are ChemMapper and the similarity ensemble technique. The toxicity of a small molecule is predicted in toxicity testing using Deep Tox, eToxPred, TargeTox, and PrOCTOR.

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